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A framework for model-based optimization of bioprocesses under uncertainty: Identifying critical parameters and operating variables.

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Abstract

The feasible production of second generation (2G) biofuels from lignocellulosic biomass as feedstock is still facing some problems both from a technical and an economical point of view (Sims et al., 2010). Despite those problems, a number of countries led by USA and EU have established ambitious targets for increasing the share of renewable energy in the transport sector (e.g. EU set a minimum of 10% of biofuels as liquid transport fuel by 2020 under Directive 2003/30/EC) (Dal Mas et al., 2010). Therefore, to overcome all these challenges, it is necessary to speed up the technological development and among others optimize the process operation. Process optimization requires identification and analysis of the most critical variables and parameters involved in the system.
What makes the process optimization a challenging task in this case is the element of uncertainties present in the system, which are a result of technological factors, operational conditions as well as economical factors. These uncertainties then lead to uncertainties in the predictions of the models of 2G bioethanol production processes, translating to uncertainties in the performance indices such as the predicted ethanol yield and unit cost. To address these uncertainties, it is required to perform a formal uncertainty and sensitivity analysis. Hence the objective of this paper is to develop and implement a systematic framework for the optimization of lignocellulosic bioethanol production under uncertainty.

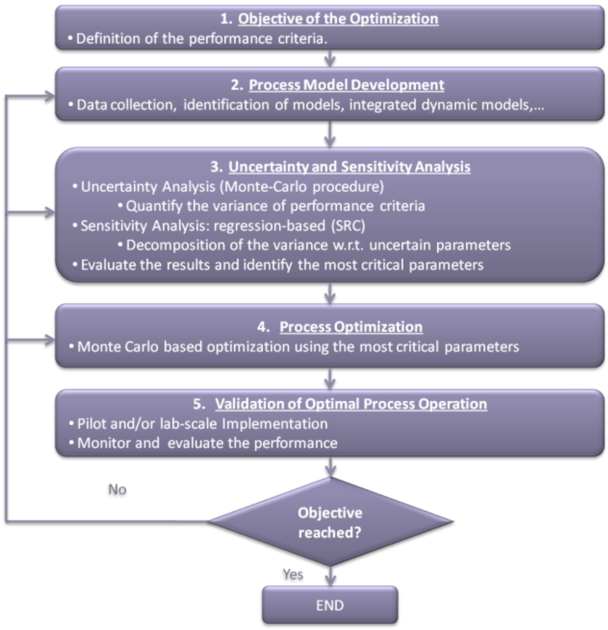

Figure 1. Systematic framework for the optimization of lignocellulosic bioethanol production under uncertainty.

The systematic framework starts with the definition of the optimization objective, followed by the collection of data, and the implementation of models (for each unit in the process) to finally develop an integrated model to describe the system. In the third step, the uncertainty and sensitivity analysis is performed to identify the critical process variables and parameters in the system. An important element here is the identification of sources of uncertainties in the system, which relies on process engineering expertise. The uncertainty analysis is then carried out using the Monte Carlo technique, which involves three steps: (i) sampling of (uncertain) parameters (Latin Hypercube Sampling), (ii) Monte-Carlo simulations with the sampled parameter values and (iii) representation of uncertainty (e.g. mean, standard deviation, variance, CDF (Helton and Davis, 2003). For the sensitivity analysis, the standardized regression coefficient (SRC) method is used, which involves building linear regression models on the output of the Monte Carlo simulations (Helton and Davis, 2003). The SRC method provides a global sensitivity measure, βi, which is a quantitative measure of how much each parameter contributes to the variance (uncertainty) of model predictions. This sensitivity measure is used as basis to identify the most critical parameters involved in the process. In the fourth step, a process optimization study is carried out by using the most critical parameters identified above. While a standard multivariable optimization method can be used (e.g., linear vs. non-linear programming), we propose a Monte-Carlo method as pragmatic and global technique to this end. In the step 5, one evaluates the performance of the optimized process operation in physical reality that is via lab or pilot-scale experiments. If the validation results are satisfactory, then the systematic procedure will be terminated. Otherwise the procedure needs to be iterated, either by reviewing the models used for the optimization or by evaluating different critical system parameters. The systematic methodology is evaluated using a number of process configurations developed in the previous study (Morales-Rodriguez et al., 2010), employing dynamic mathematical models for the involved unit operations. Preliminary results have identified the following system parameters to be the most critical parameters: enzyme loading, the acid concentration in the pre-treatment and the reactor volume in the hydrolysis and fermentation sections. The results obtained with the Monte Carlo optimization using the most critical parameters will be presented and discussed in relation to the base case.

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